Modern Spectral Analysis of Angle-Resolved Photoemission Extended Fine Structure

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INTRODUCTION

Modern spectral analysis methods have been widely used in areas involving limited-length evenly-spaced data sequences in place of the traditional direct Fourier Transforms to enhance spectral resolution and signal detectability. We introduce some of these contemporary spectral analysis techniques into Angle-Resolved Photoemission Extended Fine Structure (ARPEFS), and show that they can be a powerful tool in understanding surface structures.

REVIEW OF IMPLEMENTED METHODS

Currently we have written computer programs for four different modern spectral analysis methods (Fig.1): AutoRegression-Linear Prediction (ARLP), AutoCorrelation-AutoRegression (ACAR), AutoCorrelation-Eigenvector analysis (ACE), and Maximum Entropy Minimum Variance (MEMV). Each method has its own idiosyncrasies that we have to be careful about when applying them to analyze real world data. In our experience, we found that autocorrelation is a very good first step to enhance signal, reduce noise and stabilize the final result[1,2].

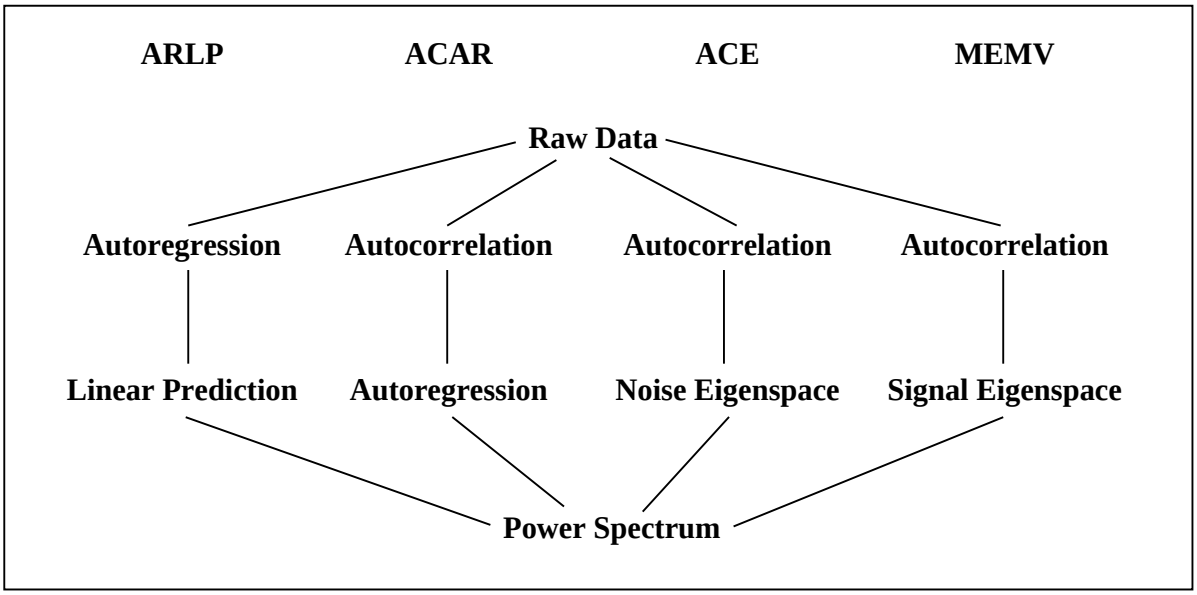

Figure 1. Flow chart comparing four modern spectral analysis methods.

APPLICATIONS

Since it was discovered that Fourier Transform of energy-scan photoelectron diffraction data yields meaningful peaks[3], people have tried to devise alternative ways to the taper-and-transform approach in the hope of finding better-looking spectra[4]. For example, in the case of ACE, we first construct an autocorrelation matrix from the raw data, then calculate the eigenvalues and their corresponding eigenvectors of this matrix. Assuming that the signals give much bigger

eigenvalues than the noises, we can single out the noise subspace that is perpendicular to the signal subspace. When we put the inner product of a harmonic with the noises in the denominator, we see a peak if the harmonic had the same frequency as one of the signals. Let's compare the performances between direct FT and ACE in the prototypical case of S/Ni(100). The picture (Fig.2) declares a clear winner.

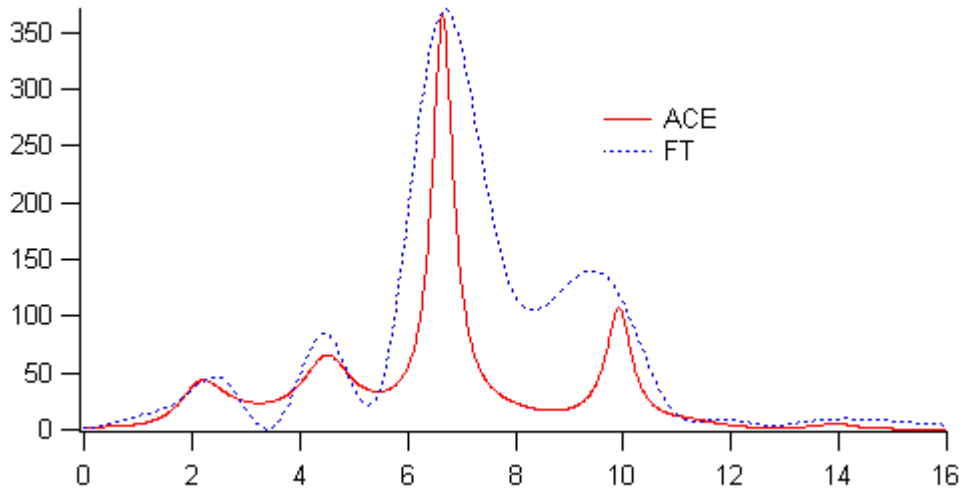

Figure 2. Power spectral density functions of normal emission S1s ARPEFS from a S/Ni(100) sample. The FT curve is obtained through a Hanning window to eliminate side-lobes and has been scaled to the same maximum height as the ACE curve. The x-axis is Path Length Difference (PLD) in Å.

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